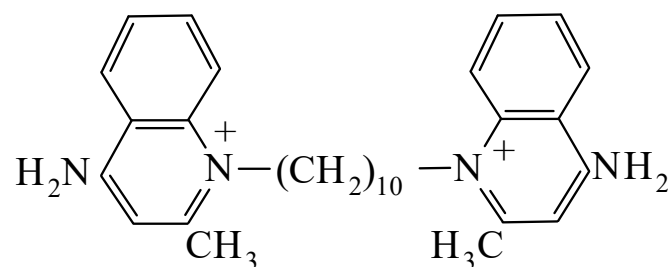




>>Entry Name: Dequalinium(2+)

Synonym(s): 1,1'-(1,10-Decanediy)[4-amino-2-methylquinolinium], 9Cl. 1,1'-Decamethylenebis[4-aminoquinaldinium], 8Cl



CAS Registry Number: 6707-58-0

Molecular Formula: $C_{30}H_{40}N_4^{2(+)}$

Molecular Weight: 456.673

Accurate Mass: 456.325296

Percentage Composition: C 78.90%; H 8.83%; N 12.27%

Calculated Log P Data: Log P 1.45 (uncertain value) (calc)

>>Derivative: Dichloride

Synonym(s): Dequalinium chloride, BAN, INN. Natralinium chloride. Dequadin. Labosept

CAS Registry Number: 522-51-0

Molecular Formula: $C_{30}H_{40}Cl_2N_4$

Molecular Weight: 527.578

Accurate Mass: 526.263

Percentage Composition: C 68.30%; H 7.64%; Cl 13.44%; N 10.62%

Use/Importance: Antibacterial agent

Physical Description: Cryst. (EtOH)

Melting Point: Mp 326 dec.°

Hazard & Toxicity: LD₅₀ (mus, scu) 70 mg/kg

Aldrich: 39992-2

Fluka: 31183

Rare Chemicals Library: S39229-4

Sigma: D3768

>>Derivative: Diacetate

Synonym(s): Dequalinium acetate. Decalinium acetate, JAN

CAS Registry Number: 4028-98-2

Molecular Formula: $C_{34}H_{46}N_4O_4$

Molecular Weight: 574.762

Accurate Mass: 574.351906

Percentage Composition: C 71.05%; H 8.07%; N 9.75%; O 11.13%

Use/Importance: Antiseptic, antifungal

Sigma: D0163

References:

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Burgess, G.G., *Aust. J. Pharm.*, 1959, **40**, 39

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Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 7876, (*synonyms*)

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